

3413-Pos Board B518**Dynamics of Red Blood Cells and Vesicles in Microchannels of Oscillating Width**

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We have studied the dynamics of red blood cells and fluid lipid vesicles in hydrodynamic flow fields created by microchannels with periodically varying channels width. For red blood cells we find a transition from a regime with oscillating tilt angle and fixed shape to a regime with oscillating shape with increasing flow velocity. We have determined the crossover to occur at a critical ratio of channel width L_y and red blood cell velocity v_m approx. $10 \pm 3s$. These oscillations are superposed by shape transitions from a discocyte to a slipper shape at low velocities and a slipper to parachute transition at high flow velocities.

Ref.:

H. Noguchi, G. Gompper, L. Schmid, A. Wixforth, T. Franke, EPL (Europhysics Letters) 2010, 89, 28002

S. Braunmueller, L. Schmid, T. Franke J.Phys. Condens. Matt. accepted

3414-Pos Board B519**Modulation of the Solid-Ordered/Liquid-Disordered Melting Temperature in *Staphylococcus Aureus* during Biofilm Formation**

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Bacteria that interact with surfaces under hydrated conditions can form aggregated structures known as biofilms. Biofilms are characterized by having increased resistance to a variety of antibacterial agents. This resistance is responsible for the generation of persistent chronic infections, and represents a serious threat to human health. Several antimicrobial agents, including hydrolytic enzymes such as PLA₂-IIA and antimicrobial peptides (AMPs) such as Magainin-2, act by disrupting bilayer membrane integrity. Since these antimicrobial agents require physical disruption of the bilayer membrane, their activity is likely to be sensitive to lipid packing. This points to a possible mechanism for generating resistance during biofilm formation through the modulation of lipid packing. Bacterial membranes present broad but cooperative lipid chain-melting events, where the membrane transitions from a solid-ordered (so) state, characterized by a high level of lipid packing, into a liquid-disordered (ld) state. For example, for *Staphylococcus aureus* (*Sa*) in planktonic state, this melting event occurs at 15°C. We have recently shown that, for *Sa*, the solid-ordered phase provides resistance towards PLA₂-IIA. In this work we show, by measuring generalized polarization of Laurdan incorporated into lipid extracts, that the position of this melting event is shifted to 28°C during *Sa* biofilm formation. Additionally, we present evidence that this shift in the melting temperature modulates resistance towards PLA₂-IIA and magainin-2. These results point to a mechanism by which bacterial membranes can generate resistance towards membrane active antibacterial agents through the modulation of the so/ld chain melting event during biofilm formation.

3415-Pos Board B520**Outer Membrane Protein Dynamics in *E.coli***

Joseph Goose, Mark S.P. Sansom.

The vast majority of currently structurally characterised outer membrane proteins of *E.coli* are beta barrel porins that exist either as monomers or homooligomers. The function of these porins is varied and complex and is thought to depend not just on their structural dynamics but also on interactions both with other porins and with their lipid environment.

To provide an insight into these processes we study in detail the motion and arrangement of both lipids and proteins within a series of model systems.

We represent the outer membrane as a bilayer consisting of mixtures of phosphatidylglycerol (PG) and phosphatidylethanolamine (PE) lipids and examine by means of atomistic and coarse grained simulations the relative dynamics of a representative sample of outer membrane proteins. We consider the diffusive ability of both isolated, and multiple proteins within larger systems which more realistically reflects the density of porins within the outer membrane. The diffusive behaviour of proteins is related to protein characteristics such as size and localised bilayer deformation.

3416-Pos Board B521**Influence of Borna Disease Virus Matrix Protein on Model Membranes Investigated by Molecular Dynamics Simulations**

Bjoern E.S. Olausson, Alexander Vogel.

Borna disease virus (BDV) is an infectious, neurotropic, enveloped RNA virus with a wide host range among the warm-blooded animals. It belongs to the *Mononegavirales* which also include Ebola and Marburg. Depending on the infected host species, BDV can influence the behavior, neural plasticity, or trigger an immunopathological reaction with high mortality rates. Although the hypothesis that BDV can infect humans is discussed very controversially, it still serves as a model for persistent viral infections in the central nervous system.

The BDV matrix protein (BDV-M) with ~16kDa is the smallest matrix protein among the negative stranded viruses. It plays an important role during the virus assembly and budding process by interacting with the host membrane and possibly the viral RNA. Studies, using a monolayer technique, showed that BDV-M condenses the lipid monolayer. Therefore, based on the 3D-structure, derived from X-Ray crystallography, a computer model was built to investigate the protein membrane interaction. The membrane consisted of POPS, POPC and Cholesterol (molar ratio 1:2:2) to closely match the brain lipid composition in terms of lipid head group charge distribution. The simulation was conducted at 303K in the NPγT ensemble and the membrane surface tension was adjusted to resemble the average order parameter measured by ²H solid state NMR to ensure the correct area per lipid. Analysis of the MD simulation showed a distinct influence on lipid diffusion rates and lipid distribution in the BDV-M facing membrane leaflet. BDV-M quickly starts sorting charged lipids beneath itself and thereby partially separates POPS from POPC. This is accompanied by an increase in the POPS diffusion rate which for the proximal interface is higher (~1.4E-06 cm²/s) compared to the distal interface (0.8E-06 cm²/s) in the first few hundred ns.

3417-Pos Board B522**Dynamics of Multicomponent Lipid Membranes at Long Length and Time Scales: Domain Growth, Rheology, and Scaling Laws**

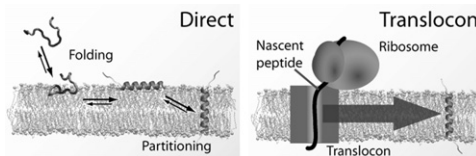
Brian A. Camley, Frank L.H. Brown.

We present a simple continuum simulation method for multicomponent lipid bilayers that accounts for both the Saffman-Delbruck hydrodynamics of the membrane and the appropriate thermal fluctuations. We use this scheme to describe the dynamics of ternary model membranes on length scales from nanometers to microns and time scales of up to tens of seconds. Simulation results for phase separation, domain diffusion, and domain flickering are all in agreement with experimental results and well-established theory. Our results also provide a simple technique to extend fluorescence microscopy "flicker spectroscopy" to determine membrane viscosities. We also study the problem of phase separation (domain growth). Simple scaling theories, along with our simulations, allow us to explain the range of scaling exponents (0.15 - 0.67) previously reported by both experiments and simulations, and provide a framework for interpreting measured coarsening exponents. We briefly address some applications of this work to biophysical models of lipid rafts, as well as extensions to systems with embedded proteins and curvature-composition coupling.

3418-Pos Board B523**Peptide Transfer Energetics from Direct Water-To-Membrane Partitioning Simulations**

Martin B. Ulmschneider.

Polypeptide partitioning properties are at the heart of biological membrane phenomena, and their precise quantification is vital for ab-initio structure prediction. However, this has proved difficult to measure experimentally. Recently the cellular translocon machinery has been employed to determine the insertion energetics for a series of systematically designed peptides. We show here that the insertion propensity, pathway and transfer energetics of these peptides into POPC bilayers can also be obtained by direct atomic resolution partitioning simulations. Remarkably, the results are in close agreement the translocon experiments, but reveal a systematic shift towards the insertion of shorter peptides. The insertion probability as a function of peptide length follows two-state Boltzmann statistics and reveal many hitherto unknown atomic-resolution details about the partitioning process. The method presented provides a powerful new tool for rapid determination of water-to-bilayer transfer properties of membrane active peptides.

**3419-Pos Board B524****Assessing Perturbations of a Fluorescent Lipid in a DPPC Bilayer with Molecular Dynamics**

David Ackerman, Jonathan Amazon, Fred Heberle, Gerald Feigenson.

Fluorescent lipid analogs are a valuable tool for studying membranes, and in recent years a wide variety of fluorescence techniques have contributed significantly to our understanding of lateral heterogeneity in both model and cell membranes. Despite their usefulness, it is often overlooked that these fluorescent molecules are extrinsic to the system of interest, and a meaningful interpretation of data, e.g. properties of nanoscopic domains, local motion and order of the probe environment, or Forster resonance energy transfer, can